

GEOMETRIC ASPECTS OF SINGULAR DISLOCATIONS

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ABSTRACT. The theory of singular dislocations is placed within the framework of the theory of continuous dislocations using de Rham currents. For a general n -dimensional manifold, an $(n-1)$ -current describes a local layering structure and its boundary in the sense of currents represents the structure of the dislocations. Frank's rules for dislocations follow naturally from the nilpotency of the boundary operator.

1. INTRODUCTION

The aim of this work is to establish a precise relationship between the theory of continuous distributions of defects and its discrete counterpart. Historically, the latter was developed first by pioneers like Volterra and Somigliana. The continuous theory was arrived at later by, among others, Bilby [BBS55], Kröner [Krö59], Kondo [Kon55] and Noll [Nol67]. Methodologically speaking, the passage from the discrete to the continuous theory was perhaps spurred by the realization that certain differential geometric objects already provide a heuristic path to generalize the discrete, intuitively graspable, picture. The clearest example is provided by the lack of closure of a Burgers' circuit enclosing an edge dislocation in two dimensions. The picture of this event so much resembles that of the lack of commutativity of two vector fields, that one would be remiss to ignore the analogy. And, in fact, the analogy is in this case fully justifiable on physical grounds. In the infinitesimal limit, the lack of closure alluded to above is a lack of integrability, whose intensity is measured by the torsion of a distant parallelism associated with the smeared-out underlying crystal lattice. Once this particular instance was exploited, the temptation could not be resisted to attribute some putative physical meaning to all kinds of other geometric objects, from Riemann curvatures to Einstein tensors. The works of Kondo and, later, Noll inaugurated the emergence of the opposite paradigm. Instead of building the theory, as it were, from the bottom up, they adopted the puristic tenet that the presence of defects (or inhomogeneities) in a continuum should be encoded automatically within the constitutive equations

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of the body and only there, without any spurious intervention of an atomic substrate. The two approaches do not necessarily lead to the same results.

Since both approaches mentioned above have undeniable merits, it would be futile to argue for one to the exclusion of the other. Our intention is, therefore, to place the theory of singular dislocations, *i.e.*, dislocations that are concentrated rather than distributed continuously, within the elegant framework of the smooth theory and so to come full circle to the original physical picture. The mathematical tool for this purpose consists of a weak reinterpretation of the differential geometric objects of the smooth theory in terms of the geometric theory of de Rham currents [dR84, Fed69].

The framework presented below applies to general manifolds. In particular, no Riemannian structure is assumed. The theory of integration of differential forms on manifolds is used throughout and the necessary background may be found in [Eps10, Seg12] within the context of continuum mechanics and in standard references on differential geometry, such as those cited therein. Specifically, for the smooth case, we consider a local layering of the material as represented geometrically by a 1-form φ , the layering form, on a manifold \mathcal{M} which may represent a material body or its image under a configuration in space. The condition that the body contains no dislocations is thus represented mathematically by the local integrability condition $d\varphi = 0$. This condition implies that at least locally (and also globally if \mathcal{M} is contractible to a point) φ is the gradient of a function u . The layers, *i.e.*, hypersurfaces of constant values of u , may be thought of as deformed Bravais planes of a crystalline body. Dislocations are present in regions where $d\varphi \neq 0$ so that such a system of layers is not available.

In the non-smooth situation, we generalize the layering 1-form to a de Rham $(n - 1)$ -current T and the condition for the body to have no dislocations is generalized to $\partial T = 0$, *i.e.*, that the boundary of the current vanishes. It is noted that in his exposition on singularities in the deformations of solids, Cermelli [Cer99] makes use of de Rham currents.

It is interesting to note that the language of differential forms and currents rather than that of frame fields, enables one to analyze dislocations associated with a single layering form or current (rather than three). From the physical point of view this means that a single family of Bravais planes is sufficient for the study of the possible presence of dislocations. It is also noteworthy that Frank's conservation rule* follows naturally from a basic mathematical property of currents, specifically, the vanishing of the boundary of a boundary.

*In the words of [Rea53, p. 34], Frank's rules are: 1. "The Burgers vector is conserved along a dislocation"; 2. "The sum of the Burgers vectors of the dislocations meeting at a node must vanish."

2. THE SMOOTH THEORY OF CRYSTAL DISLOCATIONS

2.1. Frames and coframes. The simplest theory of continuous distributions of dislocations assumes that a material body \mathcal{B} is endowed with a distinguished smooth field of bases of its tangent spaces. In general, for an n -dimensional manifold \mathcal{M} , such a field can be regarded as a section σ of the frame bundle $F\mathcal{M}$, namely

$$\begin{aligned} \sigma : \mathcal{M} &\longrightarrow F\mathcal{M} \\ x &\longmapsto \sigma(x) = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}, \end{aligned} \quad (2.1)$$

with $\pi \circ \sigma = \text{id}_{\mathcal{M}}$, where π is the bundle projection and $\text{id}_{\mathcal{M}}$ is the identity map in \mathcal{M} . We remark that smooth, or even continuous, global sections may not exist in general. A manifold for which a smooth section of $F\mathcal{M}$ does exist is said to be *parallelizable*, and the field of basis induces a *teleparallelism* (or *distant parallelism*) in the manifold.

There is an alternative (dual) way to look at a distant parallelism. Indeed, any *frame* (that is, any basis of the tangent space $T_x\mathcal{M}$) induces a unique dual basis (or *coframe*) of the cotangent space $T_x^*\mathcal{M}$, and vice versa. Therefore, a distant parallelism can also be seen as the choice of a particular coframe field. Put differently, a distant parallelism induces an \mathbb{R}^n -valued one-form on \mathcal{M} . Moreover, this coframe field can be regarded as a cross section σ^* of the coframe bundle of \mathcal{M} .

Let x^i ($i = 1, \dots, n$) be a coordinate system. Then, the frame field is given by:

$$\mathbf{e}_\alpha = e^i_\alpha \frac{\partial}{\partial x^i}, \quad \alpha = 1, \dots, n, \quad (2.2)$$

where the matrix with entries $e^i_\alpha = e^i_\alpha(x^1, \dots, x^n)$ is nowhere singular. Accordingly, the corresponding coframe is given by

$$\mathbf{e}^\alpha = e^\alpha_i dx^i, \quad \alpha = 1, \dots, n, \quad (2.3)$$

where e^α_i are the entries of the inverse matrix. As already pointed out, a coframe is clearly represented as a collection of n pointwise linearly independent 1-forms indexed by α .

2.2. The interpretation of covectors as Bravais hyperplanes. Covectors may be used to describe geometrically collections of hyperplanes. Let \mathbf{W} be a finite dimensional vector space and let $f \in \mathbf{W}^*$ be a covector, that is, a linear functional $f : \mathbf{W} \rightarrow \mathbb{R}$. Then, f may be identified uniquely with the collection H_{f1} of vectors w in \mathbf{W} such that $f(w) = 1$. This collection of vectors constitutes a hyperplane. The difference between any two elements of H_{f1} belongs to the kernel H_{f0} of the operator f . Clearly, parallel hyperplanes H_{fk} will be obtained if we consider the elements $w \in \mathbf{W}$ such that $f(w) = k$ for any integer k . Conversely, for any $w \in \mathbf{W}$, $f(w)$ may be interpreted as the amount of hyperplanes that the arrow representing w penetrates. If a covector is multiplied by a positive number a , the density of the planes is multiplied by a . A covector includes a choice of orientation

for the various planes (a positive side versus a negative side of a plane) and the multiplication of f by -1 reverses the orientation.

It is natural therefore, to use a covector as a continuous model of a system of parallel planes in a crystal (Bravais) lattice. In fact, if $\mathbf{W} = \mathbb{R}^3$, for a covector f given as

$$f = f_j dx^j, \quad (2.4)$$

relative to the standard dual basis dx^i , the components (f_1, f_2, f_3) are proportional to the Miller indices for the system of parallel planes. Whereas the Miller indices are normalized to provide a direction only, the covector f contains additional information as to the density of the layers. Let n be the dimension of \mathbf{W} . Then, a collection of n linearly independent covectors $\{f^\alpha\}$, $\alpha = 1, \dots, n$, induces a collection of n families of parallel hyperplanes. These covectors, therefore, represent a Bravais lattice.

So far we considered a single vector space \mathbf{W} . On a manifold \mathcal{M} , the interpretation just described can be applied in a point-wise manner, that is, to each tangent space $T_x \mathcal{M}$. Thus, at each point $x \in \mathcal{M}$, the covector representing the “direction” and density of the layers is given by the value $\phi(x)$ of a 1-form $\phi : \mathcal{M} \rightarrow T^* \mathcal{M}$. Noting that this setting does not require any additional structure, metric or otherwise, it is natural to study the geometric properties of such a differential form as a representation of the structure of a class of layers in a lattice. We will refer to such a form as a *local layering form*.

2.3. Integrability.

2.3.1. Intuitive considerations . Let $\mathbf{F}(x) = F^i(x) \mathbf{e}_i$ be a vector field in a 3-dimensional Euclidean vector space with Cartesian coordinates (x^1, x^2, x^3) , where $\{\mathbf{e}_i\}$ is an orthonormal basis. We recall that the condition that the vector field be conservative, namely, that there exists a scalar potential function $u(x)$ such that

$$F^i = \frac{\partial u}{\partial x^i}, \quad (2.5)$$

is

$$\frac{\partial F^i}{\partial x^j} - \frac{\partial F^j}{\partial x^i} = 0, \quad (2.6)$$

for all $i, j = 1, 2, 3$. The above well-known scheme may be generalized to an arbitrary differentiable manifold \mathcal{M} using the terminology of differential forms. In particular, one says that a differentiable r -form ϕ is *exact* if there is an $(r-1)$ -form α such that $\phi = d\alpha$, where d denotes the *exterior differentiation* of forms. Thus, α is a potential form for ϕ . Every exact form ϕ is automatically *closed*, that is $d\phi = 0$, since the d operator enjoys the property $d^2 = 0$. Conversely, if the manifold \mathcal{M} is *contractible to a point*, every closed form ϕ is exact, that is, derives from a potential. In the general case, when the manifold is not necessarily contractible to a point, if ϕ is closed, for each $x \in \mathcal{M}$ there is a neighborhood where ϕ is exact. Thus, the

condition that the form be closed is a generalization of the condition (2.6) for the existence of a local potential.

In particular, a 1-form ϕ on an n -dimensional manifold \mathcal{M} has n components, just as a vector field. Let ϕ be represented locally as

$$\phi = \phi_i dx^i, \quad (2.7)$$

where now x^i is a manifold coordinate patch. Its exterior derivative is the 2-form $d\phi$ represented locally by

$$\begin{aligned} d\phi &= \sum_{i,j} \phi_{i,j} dx^j \wedge dx^i = \frac{1}{2} \left(\sum_{i,j} \phi_{i,j} dx^j \wedge dx^i + \sum_{i,j} \phi_{j,i} dx^i \wedge dx^j \right), \\ &= \frac{1}{2} \left(\sum_{i,j} \phi_{i,j} dx^j \wedge dx^i - \sum_{i,j} \phi_{j,i} dx^j \wedge dx^i \right), \quad (2.8) \\ &= \frac{1}{2} \sum_{i,j} (\phi_{i,j} - \phi_{j,i}) dx^j \wedge dx^i, \end{aligned}$$

where commas indicate partial derivatives. Thus, the condition $d\phi = 0$ is the analog

$$\phi_{i,j} - \phi_{j,i} = 0 \quad (2.9)$$

of Equation (2.6).

We conclude that a closed 1-form represents a locally coherent collection of layers that may be identified with deformed lattice planes. In general, the 2-form $\delta = d\varphi$ is a measure of the nature of dislocation density and we will refer to it as the *dislocation density form*.

Let Z be a 2-dimensional manifold of \mathcal{M} with boundary $Y = \partial Z$. Then, by Stokes' theorem

$$I = \int_Y \varphi = \int_Z \delta \quad (2.10)$$

It follows that $\int_Y \varphi$ is independent of the particular submanifold Z . If there exists a submanifold Z_0 on which $d\varphi = 0$, *i.e.*, there are no dislocations on Z_0 , then, $\int_Z \delta = 0$ for any other submanifold Z with boundary Y , even if Z passes through a region where dislocations exist (*i.e.*, $\delta \neq 0$). In the general case where no such manifold Z_0 exists, $\int_Z \delta$ is still independent of Z , and I above is a measure the total dislocation embraced by Y in analogy with the Burgers vector.

2.3.2. Parallelism and coordinate systems. In the definition of our distant parallelism, the differentiability of the cross section has played no role whatsoever. If, on the other hand, σ^* is differentiable, we may calculate its exterior derivative $d\sigma^*$. In components, we obtain

$$\tau^\alpha = d\mathbf{e}^\alpha = e^\alpha_{i,j} dx^j \wedge dx^i, \quad \alpha = 1, \dots, n, \quad (2.11)$$

namely, $\tau = d\sigma^*$ is an \mathbb{R}^n -valued two-form which we call the *torsion of the parallelism*.[†] The identical vanishing of the torsion form, namely,

$$\tau_{ij}^\alpha = 0 \quad \alpha, i, j = 1, \dots, n, \quad (2.12)$$

is necessary and sufficient for the existence of a local coordinate system such that the original frame field σ becomes its natural base. From the point of view of the theory of dislocations in continuous media, if the frames represent crystalline bases, the vanishing of the torsion implies that the body can be smoothly brought to a configuration in which all crystal bases within a coordinate patch are mutually parallel, so that there are no defects in the lattice. The body is then *locally homogeneous*. Conversely, a non-vanishing torsion is an indication, and perhaps a measure, of the dislocation density (or *inhomogeneity*). For comprehensive treatments of the general theory of inhomogeneity see *e.g.*, [Wan67, EE07].

In the Bravais-lattice interpretation of Section 2.2, one may ask whether, given a 1-form ϕ , there is a “potential” function $u : \mathcal{M} \rightarrow \mathbb{R}$ such that $\phi = du$, where d denotes the exterior derivative (which is identical to the gradient in this situation). Such a potential function, if it exists, will label the various layers, at least locally. Indeed, these layers would be precisely the (local) level surfaces of this potential. If each one of a collection of n 1-forms $\{\phi^\alpha\}$, whose values at each point $x \in \mathcal{M}$ are linearly independent covectors, derives from a local potential function u^α , the values $u^\alpha(x_0)$ represent a point $x_0 \in \mathcal{M}$ uniquely and the body has acquired locally the crystalline structure of a perfect (non-dislocated) Bravais lattice. Recalling that the condition for the existence of a local potential u^α for a 1-form ϕ^α is the equality of the cross-derivatives, *i.e.*,

$$\frac{\partial \phi_i^\alpha}{\partial x^j} = \frac{\partial \phi_j^\alpha}{\partial x^i}, \quad (2.13)$$

we recover the integrability condition (2.12).

As just indicated, the vanishing of the torsion forms τ_{ij}^α is necessary for the integrability (holonomicity, homogeneity) of the coframe field \mathbf{e}^α . In terms of the original frame field \mathbf{e}_α , on the other hand, it is well known that the existence of an adapted coordinate system is guaranteed by the commutativity of each pair of base vector fields, namely,

$$L_{\mathbf{e}_\alpha} \mathbf{e}_\beta = [\mathbf{e}_\alpha, \mathbf{e}_\beta] = 0, \quad (2.14)$$

where $L_{\mathbf{u}} \mathbf{v}$ is the *Lie derivative* of the vector field \mathbf{v} in the direction of the vector field \mathbf{u} and where $[\mathbf{u}, \mathbf{v}]$ denotes their *Lie bracket*. In terms of components, this can be written as

$$\frac{\partial e_\beta^i}{\partial x^j} e_\alpha^j - \frac{\partial e_\alpha^i}{\partial x^j} e_\beta^j = 0. \quad (2.15)$$

[†]Notice an inessential difference with the usual definition, whereby the form takes values in $T_x \mathcal{M}$ rather than in \mathbb{R}^3 .

Since

$$0 = \frac{\partial(e_\beta^i e_j^\beta)}{\partial x^k} = \frac{\partial e_\beta^i}{\partial x^k} e_j^\beta + \frac{e_j^\beta}{\partial x^k} e_\beta^i, \quad (2.16)$$

the Lie bracket can be expressed as

$$[\mathbf{e}_\alpha, \mathbf{e}_\beta] = \left(\tau_{ij}^\sigma e_\alpha^i e_\beta^j \right) \mathbf{e}_\sigma. \quad (2.17)$$

In the context of dislocations, we may identify the Lie bracket between the two base vector fields \mathbf{e}_α and \mathbf{e}_β as the local *Burgers vector* $\mathbf{B}_{\alpha\beta}$ between the corresponding crystal directions. Expressing the Burgers vector $\mathbf{B}_{\alpha\beta}$ in the local basis, we may distinguish between the *edge component* of the dislocation density and its *screw component*, the former being the part contained in the plane spanned by the base vectors \mathbf{e}_α and \mathbf{e}_β .

2.4. Frank's rule as the vanishing of the boundary of a boundary.

Starting from the notions of simplices and chains in an affine space and their generalization to manifolds, one arrives at a fundamental geometrical and topological result of clear intuitive meaning. It states that the boundary ∂U of any well-defined domain of integration U must necessarily have a vanishing boundary, namely,

$$\partial^2 U = \partial \partial U = 0. \quad (2.18)$$

In the theory of smooth differential forms, on the other hand, the operation of exterior differentiation enjoys a formally similar property, namely, for any differential form ω on a manifold

$$d^2 \omega = dd\omega = 0. \quad (2.19)$$

The relation and consistency between these two identities is mediated by *Stokes' theorem*,

$$\int_U d\omega = \int_{\partial U} \omega, \quad (2.20)$$

where ω is an arbitrary $(p-1)$ -form and U is an arbitrary p -dimensional domain of integration.

We will presently show that a smooth version of Frank's rule for dislocation branching, [Fra51] (see also [Rea53]), can be obtained as a direct consequence of these purely geometric identities. For dimension 3, we observe that, since for any given smooth coframe field \mathbf{e}^α the torsion $\tau^\alpha = d\mathbf{e}^\alpha$ consists of 3 exact 2-forms, the integral of the torsion over the boundary of any 3-dimensional domain of integration U vanishes,

$$\int_{\partial U} \tau^\alpha = 0. \quad (2.21)$$

In the physical interpretation, this implies that there are no isolated dislocation sources, not even as a smoothed-out approximation. In particular, consider a tubular domain U and an arbitrarily small neighborhood V of U such that the torsion vanishes in $V \setminus U$, then, if we intercept U transversely

by means of two (oppositely oriented) lids Σ_1 and Σ_2 giving rise to a finite tube \hat{U} , we obtain

$$0 = \int_{\hat{U}} d\tau^\alpha = \int_{\partial\hat{U}} \tau^\alpha = \int_{\Sigma_1} \tau^\alpha - \int_{\Sigma_2} \tau^\alpha. \quad (2.22)$$

In other words, the integral of the torsion over any tube cross section is constant. The same reasoning can be applied to a tube with branches, thus providing the smooth version of Frank's rule. We note that the restriction of the coframe field to $V \setminus U$ consists of three closed 1-forms, by construction. But, since any curve surrounding the tube is not contractible to a point, these 1-forms are not necessarily exact. In physical terms, the body minus the tube is only locally homogeneous. Moreover, the integral along any such non-contractible curve of the coframe 1-forms gives rise to three constants, each of them exactly equal to the integral of the corresponding α -component of the torsion over any cross section.

From the heuristic point of view, as the diameter of the tube shrinks, we may impose the condition that the torsion increases proportionately so as to keep its integral over the cross section constant and thus recover the classical form of Frank's rule. The rigorous mathematical treatment of this limiting process will be handled in the sequel using the language of currents.

3. THE WEAK COUNTERPART

So as to generalize the notions just introduced, we define a *weak teleparallelism* ρ as an \mathbb{R}^n -valued *current* in the sense of de Rham [dR84, Fed69]. We recall that a de Rham r -current is a linear functional on the vector space of C^∞ differential r -forms with compact supports in \mathcal{M} such that $T(\phi) \rightarrow 0$ if the components of ϕ and all their derivatives tend to zero uniformly in the support of ϕ . A de Rham current is the natural generalization of a Schwartz distribution to manifolds where the forms ϕ are analogous to test functions. As such, currents provide a tool for the study of non-smooth, concentrated, physical phenomena, *e.g.*, dislocation lines and slip surfaces. We identify naturally an n -tuple of r -currents with an \mathbb{R}^n -valued r -current.

3.1. The current induced by a form. A 1-form φ on \mathcal{M} may be paired with a smooth $(n-1)$ -form ψ , having a compact support, to produce a real number in the form

$$\int_{\mathcal{M}} \varphi \wedge \psi. \quad (3.1)$$

Here, $\varphi \wedge \psi$ denotes the exterior product of the two forms, an n -form having a compact support which may be integrated over the n -dimensional manifold \mathcal{M} . Thus, the form φ induces a linear functional T_φ acting on the vector space of $(n-1)$ -forms of compact supports in \mathcal{M} in the form

$$T_\varphi(\psi) = \int_{\mathcal{M}} \varphi \wedge \psi. \quad (3.2)$$

If all the derivatives of the local representatives of the form ψ tend uniformly to zero in compact subsets of the domains of charts in \mathcal{M} , then $T_\varphi(\psi)$ tends to zero. It follows that T_φ is indeed an $(n-1)$ -current.

Remark 3.1. The action (3.2) may be given a physical interpretation in a different context. The 1-form φ may be interpreted as a force field per unit value of a certain extensive property. For example, as the electric field in the case where the property under consideration is the electric charge. Thus, the question whether φ is closed corresponds to the question of the existence of a potential function for the force field. The $(n-1)$ -form ψ is interpreted as the flux field of the property under consideration so that for any n -dimensional region $R \subset \mathcal{M}$,

$$\int_{\partial R} \psi \quad (3.3)$$

is interpreted as the total flux of the property through the boundary ∂R . Thus, $T_\varphi(\psi)$ in (3.2) may be interpreted as the total power expended by the force field while the transport of the property is given by the flux field ψ .

Remark 3.2. A collection of n 1-forms in \mathbb{R}^n , e.g., $\{\mathbf{e}^1, \dots, \mathbf{e}^n\}$ may be interpreted as the collection of gradients of the components of a velocity field. The corresponding velocity field will be incompatible, or contain dislocation rates, if the forms are not closed. Thus, for a collection of n $(n-1)$ -forms ψ^i the action

$$\int_{\mathcal{M}} \sum_i \mathbf{e}^i \wedge \psi^i \quad (3.4)$$

may be interpreted as the mechanical power performed by the stress matrix having the components ψ^i (each ψ^i has n components itself) on the velocity gradient.

3.2. Examples of currents in general. An $(n-1)$ -current in the form (3.2) is very special as it is induced by a smooth 1-form. As such it may be identified with the form φ . The fine topology used for the test forms enables one to define currents which are a lot less regular. Such currents, generalizing the local layering forms, will be referred to as *local layering currents*. We present below a number of examples.

3.2.1. The current induced by a form. We have seen already that a current T_φ , induced by a closed 1-form φ according to Equation (3.2), represents a locally coherent system of layers as in Section 2.3.1.

3.2.2. Incoherence at an interface. Let $\mathcal{M} = \mathbb{R}^2 = \{(x^1, x^2)\}$ and consider the 1-form

$$\varphi(x) = \begin{cases} dx^1, & x^2 < 0, \\ a dx^1, & a > 0 \in \mathbb{R}, x^2 \geq 0. \end{cases} \quad (3.5)$$

The form φ is not continuous, yet the current T_φ as in Equation (3.2) is well defined. For $x^2 < 0$, φ represents a collection of vertical layers and for

$x^2 > 0$, φ represents a collection of vertical layers that are a times more dense. Thus, the form φ describes incoherence at the interface $x^2 = 0$ for $a \neq 1$.

3.2.3. A Dirac current. Let v_1, \dots, v_{n-1} be a collection of vectors in $T_{x_0}\mathcal{M}$ for a point $x_0 \in \mathcal{M}$. Then,

$$T(\psi) = \psi(x_0)(v_1, \dots, v_{n-1}) \quad (3.6)$$

is an $(n-1)$ -current which is a generalization of the Dirac delta distribution.

3.2.4. The current induced by the exterior derivative. Consider the $(n-2)$ -current $T_{d\varphi}$ induced by a 1-form φ as

$$T_{d\varphi}(\omega) = \int_{\mathcal{M}} d\varphi \wedge \omega, \quad (3.7)$$

for any compactly supported $(n-2)$ -form ω . Using the basic property of exterior differentiation whereby

$$d(\alpha \wedge \beta) = d\alpha \wedge \beta + (-1)^r \alpha \wedge d\beta, \quad (3.8)$$

for an r -form α , Equation (3.7) may be written in the form

$$\begin{aligned} T_{d\varphi}(\omega) &= \int_{\mathcal{M}} d(\varphi \wedge \omega) + \int_{\mathcal{M}} \varphi \wedge d\omega, \\ &= \int_{\partial\mathcal{M}} \varphi \wedge \omega + \int_{\mathcal{M}} \varphi \wedge d\omega, \\ &= \int_{\mathcal{M}} \varphi \wedge d\omega, \end{aligned} \quad (3.9)$$

where in the second line we used Stokes's theorem and in the third line we used the fact that ω is compactly supported in \mathcal{M} .

3.2.5. Polyhedral chains as currents. A current T_s can be uniquely associated with an $(n-1)$ -simplex s in \mathcal{M} . It is defined as

$$T_s(\psi) = \int_s \psi, \quad (3.10)$$

for any compactly supported $(n-1)$ -form ψ . Thus, rather than a continuous system of layers modeled by a form φ as in Section 3.2.1 above, T_s represents a single “concentrated” layer. For example, a simplex s inside \mathcal{M} may represent a cut inside the body where an additional layer of atoms has been added or removed.

Evidently, we may extend this definition to an arbitrary chain $A = \sum_p a_p s_p$ and define T_A by

$$T_A(\psi) = \sum_p a_p \int_{s_p} \psi. \quad (3.11)$$

3.2.6. *The product of a current by a function.* Let T be a current and u a smooth function. Then, one may define the product current uT by

$$uT(\psi) = T(u\psi). \quad (3.12)$$

In particular, for the current T_s of the previous example,

$$uT(\psi) = \int_s u\psi. \quad (3.13)$$

3.3. **Dislocations as boundaries of currents.** We recall that the boundary of a p -current T is the $(p-1)$ -current ∂T defined by

$$\partial T(\omega) = T(d\omega). \quad (3.14)$$

In case $\partial T = 0$, one says that T is closed. Just as a current is a non-smooth generalization of the system of layers represented by a 1-form, $\partial T = 0$ is a generalization of the condition $d\varphi = 0$ (see Section 3.3.1 below) implying coherence of the system. In fact, a theorem by de Rham (see [dR84, pp. 79–80]) asserts that any closed current is homologous to a current T_φ induced by some smooth form φ , *i.e.*, there exists a current S such that for each compactly supported smooth form ψ ,

$$(T - T_\varphi)(\psi) = T(\psi) - \int_{\mathcal{M}} \varphi \wedge \psi = \partial S(\psi). \quad (3.15)$$

In other words, the homological properties of T may be obtained by the analogous properties of a current induced by an approximating smooth form φ . As the dislocation structure of a smooth form φ is obtained by $d\varphi$ and as $\partial T_\varphi = T_{d\varphi}$ (Section 3.3.1), it is natural to obtain the dislocation structure induced by the $(n-1)$ -current T from its boundary ∂T . Thus we will refer to the $(n-2)$ -current $D = \partial T$ as the *dislocation current*.

Again, we demonstrate the significance of these notions in the following examples.

3.3.1. *The boundary of a current induced by a smooth form.* Consider Section 3.2.4 above. It follows from Equation (3.9) that for a 1-form φ ,

$$\partial T_\varphi = T_{d\varphi}. \quad (3.16)$$

We conclude that if φ is closed then $\partial T_\varphi = 0$. This is just the condition for coherence phrased in terms of currents.

3.3.2. *The dislocation current for an incoherent interface.* Consider Example 2 above. Using \mathbb{R}^{2-} and \mathbb{R}^{2+} to denote the lower and upper half planes

in \mathbb{R}^2 , we have for each 0-form ω ,

$$\begin{aligned}
\partial T_\varphi(\omega) &= \int_{\mathbb{R}^{2-}} dx^1 \wedge d\omega + \int_{\mathbb{R}^{2+}} a dx^1 \wedge d\omega, \\
&= - \int_{\mathbb{R}^{2-}} d(dx^1 \wedge \omega) + \int_{\mathbb{R}^{2-}} d^2 x^2 \wedge \omega \\
&\quad - \int_{\mathbb{R}^{2+}} a d(dx^1 \wedge \omega) + \int_{\mathbb{R}^{2+}} a d^2 x^2 \wedge \omega, \\
&= - \int_{\partial \mathbb{R}^{2-}} dx^1 \wedge \omega - \int_{\partial \mathbb{R}^{2+}} a dx^1 \wedge \omega, \\
&= (a-1) \int_{\partial \mathbb{R}^{2-}} \omega dx^1,
\end{aligned} \tag{3.17}$$

where it is noted that $\partial \mathbb{R}^{2-}$ and $\partial \mathbb{R}^{2+}$ contain the set $L = \{(x^1, 0)\}$ but with opposite orientations. Let T_L be the 0-current in \mathbb{R}^2 defined by

$$T_L(\omega) = \int_{\partial \mathbb{R}^{2-}} \omega dx^1. \tag{3.18}$$

Then, the preceding calculation shows that

$$\partial T_\varphi = (a-1)T_L. \tag{3.19}$$

Indeed, for the case where $a = 1$, $\partial T_\varphi = 0$ and T_φ is a closed current which represents a coherent collection of layers. In case $a \neq 1$, the dislocations are concentrated on the line L which is the support of ∂T_φ , i.e., $\partial T_\varphi(\omega) = 0$ for any 0-form (a function) ω whose support is disjoint from L .

3.3.3. The dislocation current induced by a polyhedral chain. Referring to Section 3.2.5, we note that by Stokes's theorem,

$$\begin{aligned}
\partial T_s(\omega) &= \int_s d\omega, \\
&= \int_{\partial s} \omega,
\end{aligned} \tag{3.20}$$

so that

$$\partial T_s = T_{\partial s}, \tag{3.21}$$

where ∂s is viewed as a polyhedral chain. Thus, as one would expect, the dislocation line is the boundary of the embedded simplex. Evidently, the boundary operator is linear and may be extended in this case to a polyhedral chain.

3.3.4. General incoherent interfaces. Let Y be an n -dimensional submanifold of \mathcal{M} with boundary $Z = \partial Y$. Let φ be a closed form and consider the layering current

$$T(\psi) = \int_Y a \varphi \wedge \psi + \int_{\bar{Y}} \varphi \wedge \psi, \tag{3.22}$$

where $a > 0 \in \mathbb{R}$ and \bar{Y} is the manifold with boundary $-Z$ whose interior is $\mathcal{M} \setminus Y$ (so that the orientation of $\partial(\mathcal{M} \setminus Y)$ is the opposite of the orientation of Z). We have

$$\begin{aligned} D(\omega) &= \partial T(\omega) = \int_Y a\varphi \wedge d\omega + \int_{\bar{Y}} \varphi \wedge d\omega, \\ &= - \int_Y ad(\varphi \wedge \omega) + \int_Y ad\varphi \wedge \omega, \\ &\quad - \int_{\bar{Y}} d(\varphi \wedge \omega) + \int_{\bar{Y}} d\varphi \wedge \omega, \end{aligned} \quad (3.23)$$

and using the assumption that $d\varphi = 0$, it follows that

$$\partial T(\omega) = (1 - a) \int_Z \varphi \wedge \omega. \quad (3.24)$$

Thus, the dislocations are distributed over the boundary of Y while the material is coherent inside and outside Y .

3.3.5. A dislocation line. Consider the case where $\mathcal{M} = (-1, 1)^3$ is an open cube in \mathbb{R}^3 . Let

$$s = \{(0, x^2, x^3) \in \mathcal{M} \mid x^2 \leq 0\} \quad (3.25)$$

equipped with the orientation induced by the form $dx^2 \wedge dx^3$ and let T_s be the 2-current defined by

$$T_s(\varphi) = \int_s \varphi \quad (3.26)$$

for any 2-form φ compactly supported in \mathcal{M} . It follows that for any compactly supported 1-form ω ,

$$\begin{aligned} \partial T_s(\omega) &= \int_s d\omega, \\ &= \int_L \omega, \end{aligned} \quad (3.27)$$

where $L = \{(0, 0, x^3) \in \mathcal{M}\}$ oriented naturally by the form dx^3 . Clearly, L represents the line of dislocation associated with the half plane s . Notice how closely the layering current T_s matches the addition of a half plane of atoms as depicted in standard texts on dislocations.

3.3.6. The boundary of a product of a function and a chain. Using again the setting of Section 3.2.6, let s be an $(n-1)$ -simplex in the n -dimensional manifold \mathcal{M} and let u be a smooth function. Set

$$T_{us}(\psi) = \int_s u\psi \quad (3.28)$$

for every compactly supported $(n-1)$ -form ψ on \mathcal{M} . It follows that for every compactly supported $(n-2)$ -form ω on \mathcal{M} one has

$$\begin{aligned}
\partial T_{us}(\omega) &= T_{us}(\mathrm{d}\omega), \\
&= \int_s u \mathrm{d}\omega, \\
&= \int_s \mathrm{d}(u\omega) - \int_s \mathrm{d}u \wedge \omega, \\
&= \int_{\partial s} u\omega - \int_s \mathrm{d}u \wedge \omega, \\
&= (T_{u\partial s} - T_{s\perp} \mathrm{d}u)(\omega).
\end{aligned} \tag{3.29}$$

Here, we have used the notation

$$T_{\perp} \alpha(\omega) = T(\alpha \wedge \omega) \tag{3.30}$$

for an r -current T , a p -form α and a compactly supported smooth $(r-p)$ -form ω . Thus, in general, one has

$$\partial T_{us} = T_{u\partial s} - T_{s\perp} \mathrm{d}u. \tag{3.31}$$

Clearly, one may replace s above by a polyhedral chain or a smooth submanifold (using triangulation).

3.3.7. A node of three dislocation lines. Let $\mathcal{M} = (-1, 1)^3 \subset \mathbb{R}^3$, $s_1 = \{(0, x^2, x^3) \in \mathcal{M} \mid x^2 \leq 0, x^3 \geq 0\}$, $s_2 = \{(x^1, x^2, 0) \in \mathcal{M} \mid x^1 \geq 0, x^2 \leq 0\}$, $s_3 = \{(x^1, x^2, 0) \in \mathcal{M} \mid x^1 \leq 0, x^2 \leq 0\}$ where the quarter planes s_1, s_2, s_3 are oriented by the normals $\mathbf{n}_1 = (1, 0, 0)$, $\mathbf{n}_2 = (0, 0, 1)$ and $\mathbf{n}_3 = (0, 0, -1)$, respectively. Consider the layering described by the current

$$T = T_{a_1 s_1} + T_{a_2 s_2} + T_{a_3 s_3}, \tag{3.32}$$

so that

$$T(\psi) = \sum_{i=1}^3 a_i \int_{s_i} \psi, \tag{3.33}$$

for a smooth compactly supported 2-form ψ . Thus,

$$\begin{aligned}
D(\omega) &= \partial T(\omega), \\
&= \sum_{i=1}^3 a_i \int_{s_i} \mathrm{d}\omega, \\
&= \sum_{i=1}^3 a_i \int_{\partial s_i} \omega, \\
&= (a_1 T_{L_1} + a_2 T_{L_2} + a_3 T_{L_3} + (a_1 - a_2 - a_3) T_L)(\omega),
\end{aligned} \tag{3.34}$$

where the one dimensional simplices L_p are define as follows: L_1 is the segment from the origin to $(0, 0, 1)$, L_2 is the segment from $(1, 0, 0)$ to the origin, L_3 is the segment from $(-1, 0, 0)$ to the origin, L is the segment from $(0, -1, 0)$ to the origin. It is noted immediately that if the dislocation

current is supported only on the “fork” $L_1 \cup L_2 \cup L_3$, then, one has the condition

$$a_1 = a_2 + a_3. \quad (3.35)$$

Evidently, this result, a particular case of Frank’s second rule, will also hold if the cube is deformed under any embedding in \mathbb{R}^3 . Furthermore, the choice of planes is immaterial. (See also Section 3.4.3.)

3.4. The boundary of a boundary and Frank’s rules. The theory of currents provides a generalization of the intuitive result of combinatorial topology that the boundary of the boundary of a chain is zero. This follows immediately from

$$\partial^2 T(\alpha) = \partial T(d\alpha) = T(d^2\alpha) = 0. \quad (3.36)$$

The dislocation current D is obtained as the boundary of a current T . Hence,

$$\partial D = \partial^2 T = 0 \quad (3.37)$$

is a condition that the dislocation current must satisfy. In other words, the dislocation current must be closed.

We may use this result in the following situations.

3.4.1. Frank’s first rule. Let L be an $(n-2)$ -dimensional submanifold without boundary in the manifold \mathcal{M} . (For example, in a three dimensional situation, L could be a curve that does not have ends inside \mathcal{M} .) We assume that L is the support of the dislocation current D . We want to examine the possibility that the dislocation current is of the form

$$D = T_{uL} \quad (3.38)$$

for some real valued function u defined on \mathcal{M} . Thus, there is a local layering $(n-1)$ -current S such that

$$D = T_{uL} = \partial S. \quad (3.39)$$

Using Equation (3.31) for the submanifold L (instead of s), we have

$$\begin{aligned} 0 &= \partial D, \\ &= \partial T_{uL}, \\ &= T_{u\partial L} - T_L \lrcorner du, \end{aligned} \quad (3.40)$$

and, by the assumption that $\partial L = 0$, we conclude that

$$du = 0 \quad (3.41)$$

so that u must be constant on L . This result is clearly analogous to the Frank’s first rule (in which case L is 1-dimensional) and it is an example of the constancy theorem of geometric measure theory.

3.4.2. *Frank's first rule for the boundary of a submanifold.* Let Z be an $(n-1)$ -dimensional submanifold with boundary ∂Z of \mathcal{M} , let u be a smooth function on \mathcal{M} and consider the $(n-1)$ -current T_{uZ} given as

$$T_{uZ}(\psi) = \int_Z u\psi. \quad (3.42)$$

Using the analog of (3.31) for the submanifold Z , we have

$$\partial T_{uZ} = T_{u\partial Z} - T_Z \lrcorner du. \quad (3.43)$$

Assume that ∂T_{uZ} is supported on ∂Z . By applying ∂T_{uZ} to forms whose supports are disjoint from ∂Z , it follows that du must vanish on Z . We conclude therefore that if u is not constant on Z , the support ∂T_{uZ} contains points outside ∂Z . In the context of dislocations, if the “intensity” of the dislocations along a certain line L is not constant, there should be additional continuous dislocations on the dislocation surface Z outside L .

3.4.3. *Frank's second rule.* Let \mathcal{M} be a nonempty bounded open subset of \mathbb{R}^3 and let $A \in \mathcal{M}$. Consider 3 curves L_i , $i = 1, 2, 3$ in \mathcal{M} such that each L_i is connected in \mathcal{M} , it originates at A and is the intersection of the image of a curve $c_i : [0, 1] \rightarrow \mathbb{R}^3$ with \mathcal{M} such that $c_i(1) \notin \mathcal{M}$. (In other words, each c_i ends on the topological boundary of \mathcal{M} where it is noted that \mathcal{M} has no boundary as a manifold and not as a current.) Thus, $\partial L_i = \{A\}$ as a manifold and $\partial T_{L_i} = T_A$ (the Dirac delta) as a current. We examine the case where the dislocation current is given by $D = \sum_i a_i T_{L_i}$. It follows that for an arbitrary compactly supported smooth 0-form α ,

$$\begin{aligned} 0 &= \partial D(\alpha), \\ &= \sum_i a_i \int_{L_i} d\alpha, \\ &= \sum_i a_i \alpha(A). \end{aligned} \quad (3.44)$$

We conclude therefore that $0 = \sum a_i$. This condition is evidently analogous to Frank's second rule for dislocations.

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